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DEVELOPMENTS IN CONSEQUENCE MODELLING OF ACCIDENTAL RELEASES OF HAZARDOUS MATERIALS

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Research article

Abstract: The modelling of consequences of releases of hazardous materials in the Netherlands has mainly been based on the "Yellow Book". Although there is no updated version of this official publication, new insights have been developed during the last decades. This article will give an overview of new developments in consequence modelling, focussing on fire modelling.

Key words: Consequence modelling, BLEVE, Jet fire, Pool fire, Vapour Cloud Explosion.

Introduction

Although the Netherlands may have an established reputation for its countryside, one should be aware of the fact that this country, with many of the 16 million inhabitants concentrated in the urbanised west coast area, also has densely populated areas.

Having highly industrialised regions, including large chemical sites close to urban areas, the Netherlands were one of the first countries to start with a regulation on safety. Already in the seventies, the Dutch "Committee on the Prevention of Disasters" published the first version of the "Yellow book" (CPR 14E, 2006), describing methods for the calculation of physical effects due to releases of hazardous materials. Basically, this Yellow Book was one of the first guidelines on "How to perform a consequence analysis". As a composer of this handbook, TNO realises that providing formula's and describing methods doesn't fully answer the "is it safe enough?" question. When it comes to answering questions about local situations, or possible domino (cascading) effects, much more detailed calculations are required. Furthermore, knowledge on modelling is still developing, new (e.g. CFD based) methods became available, and insights on possible dangers (NaTech events) are improving.

Materials and methods

Consequence modelling: beyond the Yellow Book

Unfortunately, the Dutch Government, having its regulation based on the Coloured Books (CPR 14E, 2006; CPR16E, 2005; CPR 18, 2005), isn't too keen on introducing these "new insights" in consequence modelling. Adopting new insights would mean that already accepted situations would need to be re-evaluated, which may have big consequences for companies that currently have a "permit to operate" based on their safety reports. For that reason, there is hardly a driving force to establish an official "updated Yellow book" that will include improved insights in consequence modelling. Note that, although the 2nd revised print of the Yellow Book (YB) was updated in 2005, the theory itself was still based on literature from the 90's.

Because TNO also provides its "EFFECTS" consequence modelling tool to our industrial customers, we were faced with the need to update and adjust the consequence models beyond the theory available in the YB. Furthermore, because we also intensively use the models ourselves, we were well aware of limitations in the models, or potential extensions that would provide more insight in the potential accident effects. Since the last revision of the YB, organisations like American CCPS, the French INERIS, or the UK- HSE have published several papers on improved consequence models. As a result of the effort in keeping our consequence models up to date, many consequence models included in EFFECTS have already been adapted beyond the YB or models are being extended to offer more possibilities. This paper will present some examples of improved consequence modelling, focussing on fire modelling.

Results

BLEVE modelling: Dynamic BLEVE model

Because of the large number of LPG transports (both by rail and by road) and the high lethality

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levels within short distances of the transport routes, the BLEVE phenomena (Boiling Liquid Expanding Vapour Explosion) is one of the most dominating potential accident scenario's in the Netherlands. Although the YB already provides a BLEVE model which accurately predicts size, height, duration and resulting radiation of the fireball, a more recent CCPS publication by Martinsen and Marx (Martinsen and Marx, 1999) appeared to take into account the fact that the BLEVE is actually a dynamic phenomenon: the fireball will grow and rise up in the air as a function of time. The original YB model would simply assume the fireball to start at its full size and lift-off height, and be there for a number of seconds. The dynamic development of size and height will influence the resulting radiation and heat-dose, especially at short distance since the fireball starts at ground level. The dynamic BLEVE model has been already released in the current EFFECTS software. Since we believe that the dynamic BLEVE is a more realistic and better description of the heat radiation phenomenon, we advise to use this dynamic model instead of the "static" YB model. Fig. 1 illustrates the difference in max. heat flux and consequences determined by the two BLEVE models.

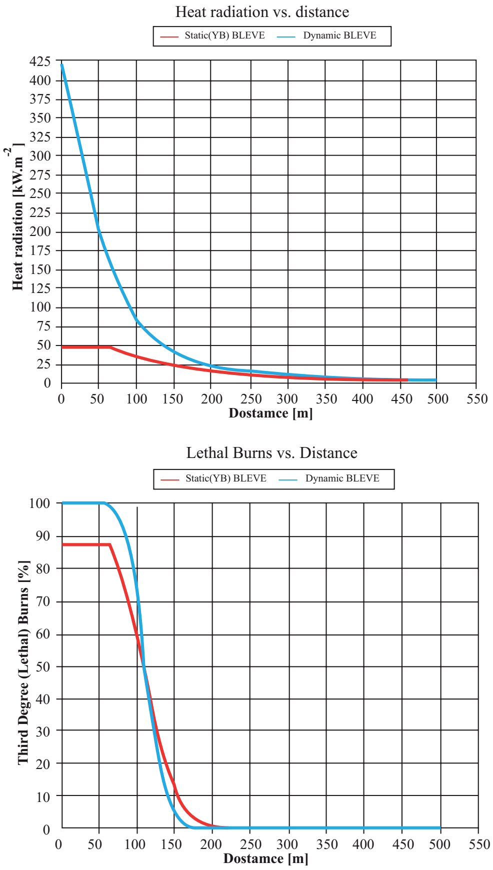

Fig. 1 Max heat radiation versus distance and lethality versus distance for Static YB BLEVE (red) versus Dynamic BLEVE (blue)

Jet fire modelling: Two Phase jet fire

The YB itself does not contain a model for jet-fires from two phase releases, such as a propane-torch. For gas-based flares, the "Chamberlain" (Chamberlain, 1987) model is generally accepted and selected in the YB, but for pressurised liquefied gasses the only available model we were using was a simple point-source model which originated from the 70's by the American Petroleum Institute. A more recent publication by Cook (Cook et al., 1990) appeared to contain verified relations to determine the size and heat radiation levels for a two-phase jet-fire. Basically, this publication provides some modifications to the single phase (gas) jet model in order to calculate the dimensions of the two phase jet flame, enabling the possibility to integrate the two-phase jet into the existing gas jet fire model.

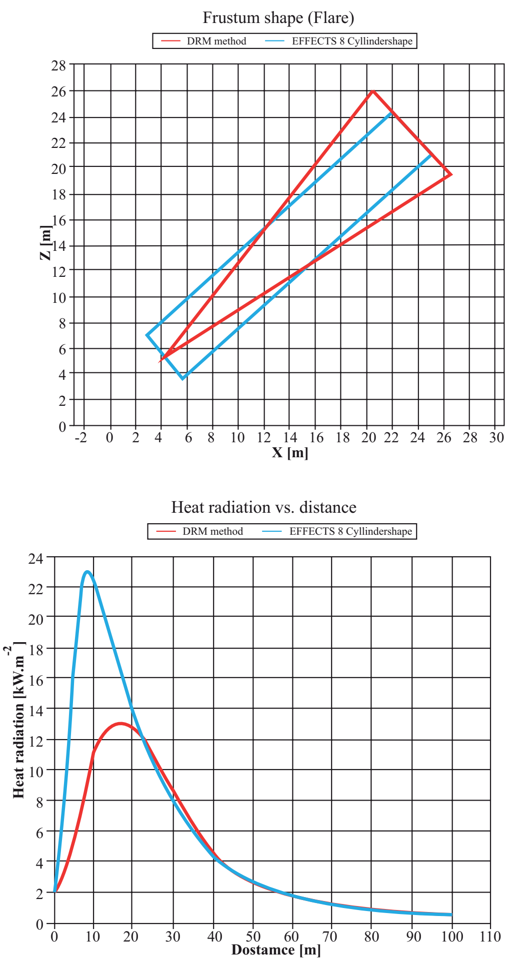

Fig. 2 Modelled shape of frustum and resulting heat radiation versus distance for YB (blue) and DRM method

Furthermore, one of the issues with calculating the heat radiation coming from a “cone shaped” flame area had to do with the way the “view factor” of the jet fire was calculated. Originally, the torch was modelled as a tilted cylinder, with an averaged diameter matching the calculated surface area of the flame. However, when dealing with non-elevated and non-vertical flames, the heat radiation at short distances was strongly influenced by this simplified cylinder shape where the bottom part of the cylinder would be close to the receiver (see Fig. 2). Instead of using derived goniometric relations for the view factor of a cylinder, the enhanced model is now using a discretized method, dividing the flame area into small surface elements, each with a unique area and orientation towards the receiving plane (see Discretized heat radiation calculation).

Pool fire modelling:Two-zone pool fire

Originally, the YB provided a straightforward model that would calculate the heat radiation of a pool fire based on chemical properties (burning speed), pool area and wind speed that would lead to a single flame height and corresponding tilting angle. Together with a “soot fraction” for which some chemical specific values were provided, this would result in heat load values around the pool fire. Recent experiments however illustrated that apart from this chemical dependent soot fraction, one could distinguish a luminous clear zone and a really fuliginous or sooty top part of the flame. This “two zone” pool fire approach was described in publications by Rew and Hubert (Rew and Hubert, 1996; Rew et al., 1997) where an extensive validation was done for a wide range of petrochemicals. Apart from differentiating a clear part, with a very high SEP (Surface Emissive Power, the heat radiation intensity), and a sooty part the flame, the model also included the effect of a flame shape elongation; the influence of the wind forcing the top of the flame into an elliptical shape.

Again, the differences with the original YB model are most explicit at shorter distances, where the clear bottom part of the flame has its highest influence. However, it is at those shorter distances were significant lethality levels may be expected (using the Green Book (CPR16E, 2005) damage relations), so the change to a “two zone pool fire model” will often lead to significant higher lethality distances as compared to a “one zone”(YB) model.

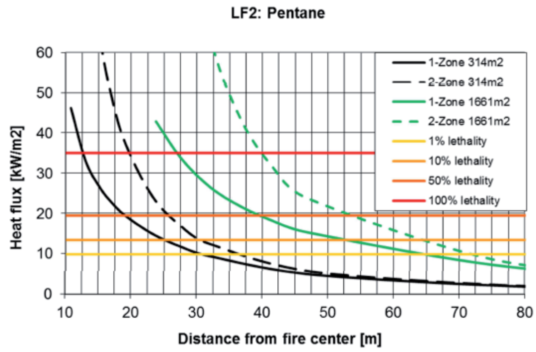

Fig. 3 Heat radiation versus distance and lethality levels for 1 zone (YB) and two-zone pool fire model for a Pentane fire

Discretized Heat Radiation calculations

The unrealistic results when modelling a tilted, non-elevated jet fire as a cylinder, and the description of the two-zone pool fire as a “sheared elliptical cylinder” clearly required adaptations in the way the view factor of a flame was calculated. Usually, the fire models use an analytically derived goniometric formula to describe the view factor of typical 3D base shapes, like view factors for cylinders or sphere’s as found in Mudan (Mudan, 1987). However, when a radiating shape is divided into multiple plane elements, the problem can be reduced to a simple plane-to-plane calculation. For such a discretized surface, the total energy radiated from a flame to a receiver surface can be expressed by the relation:

$$Q = \int_{A_f} \int_{A_r} SEP\, \tau_a \frac{\cos\beta_r \cos\beta_f}{\pi\, s^2} dA_f dA_r$$

where:

S Path length between flame and receiver,

dA_f (discretized) Area flame,

dA_r (discretized) Area receiver,

SEP Surface Emissive Power flame,

β_f Angle vector along S and normal to flame area A_f,

β_r Angle vector along S and normal to receiver area A_r,

τ_a Transmissivity of atmosphere.

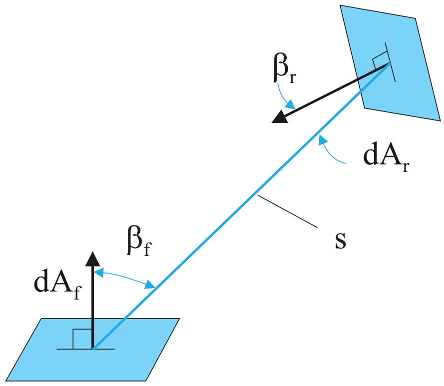

Fig. 4 Radiation heat exchange between two spatially oriented planes

Instead of using the original analytical formulas, the “sheared elliptical cylinder shaped” pool fires and “cone” shaped jet fires can be modelled as arrays of surface elements, as depicted in Fig. 5.

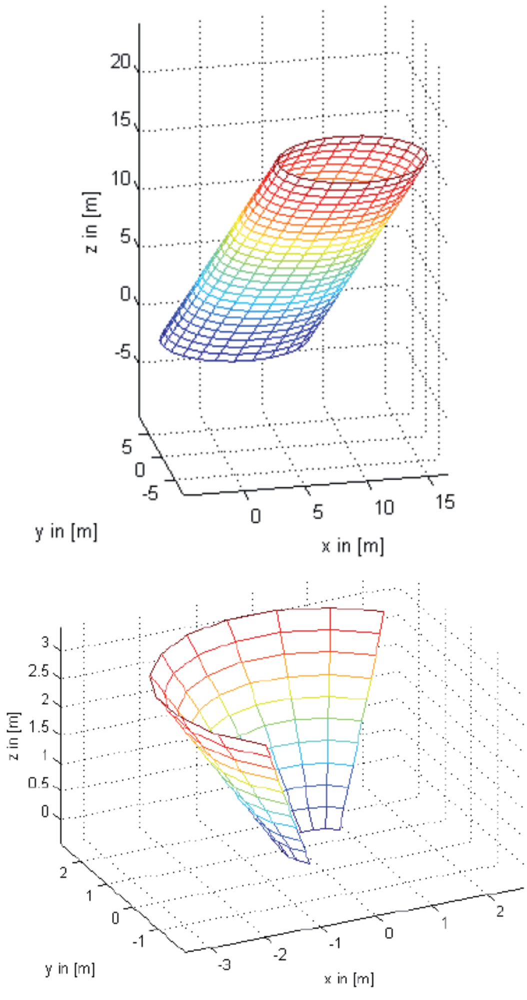

Fig. 5 Translation of a “sheared cylinder” and cone shape into surface elements

When calculating the “heat radiation footprint” of jet fires or pool fires, a typical “receiver height” is assumed, and the maximum irradiated energy at [*x*, *y*, height] is calculated by assuming $\beta_r = 0$ degrees: as if the receiver object is always facing the fire. This DRM (“Discretized Radiation Model”) is included in the new jet fire model of EFFECTS 9. The two zone pool fire models will be released in the forthcoming EFFECTS 9.1. The DRM method can also be applied to non-circular pool fire calculations, such as “Rectangular pool”, “Rim fire” and “Polygonal shaped pool”.

Domino effects: flame - receiver object calculations

When investigating the potential risks of domino effects due to heat radiation, one is often interested in the heat radiation at adjacent objects, which can be critical process equipment or other constructions sensitive to heat radiation, thus triggering a cascading event. Using the discretized geometry of the receiving construction, the DRM method and the associated relations can also be used to calculate heat load on receiving geometries.

Some examples of heat load on construction calculations are given in the Fig. 7 to Fig. 9 which were made with a stand-alone version of the DRM model. The colour scale illustrates receiving heat fluxes in [W.m^{-2}].

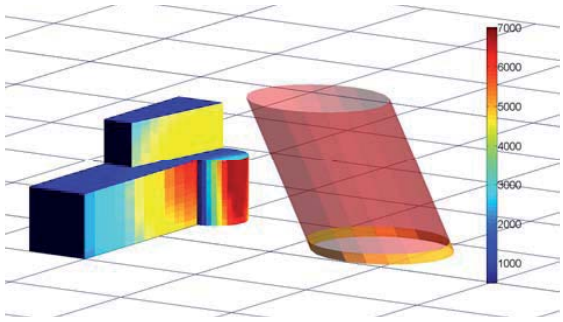

Fig. 6 Heat radiation from a (two zone) diesel pool fire received by the front of a building

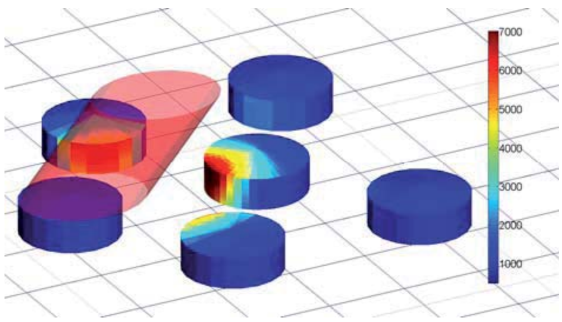

Fig. 7 Fire in an oil tank and the resulting heat flux to the adjacent tanks

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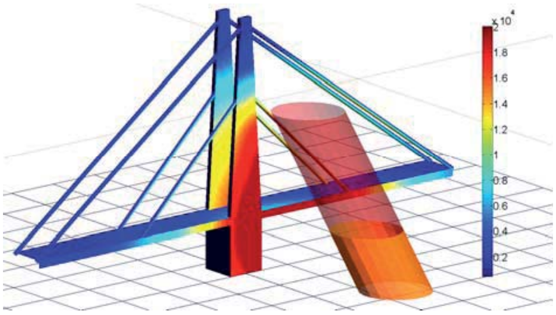

Fig. 8 Heat radiation received by a bridge from an LPG pool fire on water

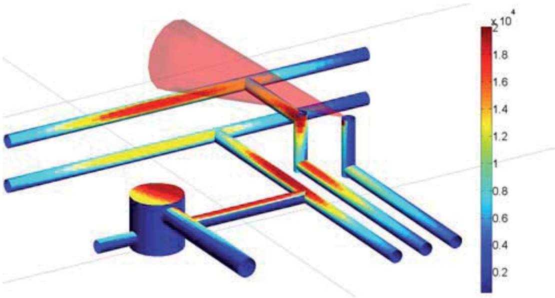

Fig. 9 Heat radiation from an LNG jet fire received by a pipeline system

Although we don't intend to supply EFFECTS with a full 3D modeller, the idea is to provide the possibility to define some standardised geometries (blocks, cylinders) to be able to evaluate heat fluxes on receiving geometries.

Domino effects: Vapour Cloud Explosions in congested areas

The potential damage of a Vapour Cloud Explosion (VCE) is generally seen as one of the most feared accident scenario in petrochemical operations. Although dedicated dispersion models may be able to calculate "explosive mass" of a cloud, and provide the size and location of a flammable cloud as a function of time, it remains difficult to predict the potential blast resulting from an explosion when a cloud gets ignited within a congested area. Several years ago, TNO already developed guidance for the application of the "Multi Energy" method (Eggen, 1998). The Multi Energy method itself has been widely used to predict the overpressure and pressure impulse resulting from VCE's, but the method requires to select a "curve number" or "blast strength category" for the explosion, and an estimation of the fraction of the cloud that is incorporated within the explosion. Instead of giving some qualitative suggestions for selecting the blast strength, the GAME relations provided a quantitative relation to correlate the initial overpressure with parameters characterising the environment in which the vapour cloud is located. For low ignition energy and no parallel plane confinement (open, 3D), this expression is:

$$P_0 = 0,84 \cdot \left(VBR \cdot L_p / D\right)^{2,75} \cdot S_L^{2,7} \cdot D^{0,7}$$

where:

P_0 The maximum explosion overpressure [bar],

VBR Volume blockage ratio [-],

L_p Length of the flame path [m],

D Typical diameter [m],

S_L Laminar burning velocity of the flammable mixture [m.s^{-1}].

The resulting maximum overpressure can be used to select the (potentially interpolated) blast strength from the original 10 sets of "Multi Energy" curves. Although the method has been available for some time, the currently available computer power allows performing iterative calculations where potential cloud locations can be projected upon "congested areas" which have specific characterising parameters. Our current effort in this field is aimed at predicting maximum overpressure (worst case) contours for specific site layout and release locations.

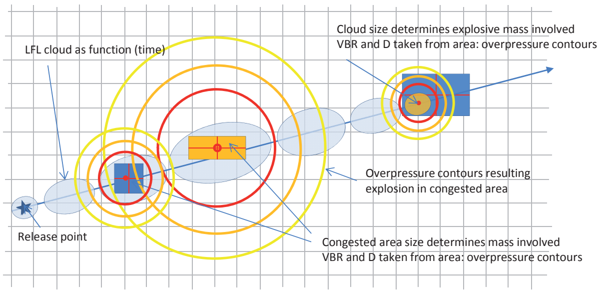

Fig. 10 Calculating overpressure contours for various potential LEL cloud locations and receiving congested areas

By evaluating various possible cloud locations, and resulting overpressure contours for various "receiving" congested areas (with potentially varying "vulnerability" or "fragility curves") , this enhanced GAME based method enables the possibility to check potential cascading effects of VCE's.

Conclusion

Although there is no governmental incentive in the Netherlands to work towards a new official "Yellow Book" we will continue adapting our consequence models to overcome shortcomings, extend possibilities and to make the predictions

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more realistic. Our effort is aimed at providing a transparent, traceable en reproducible result (not using proprietary methods) which implies that all new models will be referring to open (scientific) literature, and need to be explicitly documented and validated. Of course we can only agree on the results of models if we agree on the methods. For this reason we would like to challenge the international audience to keep publishing and thus sharing knowledge on consequence modelling. I hope this presentation and its references can be a contribution to this challenge.

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